

Methylparaben

99-76-3 | DTXSID4022529

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.06

Global applicability domain: Inside

Local applicability domain index: 7.10e-01

Confidence level: 7.63e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methyl 3-hydroxybenzoate</div> <div>Measured: 1.89</div> <div>Predicted: 2.06</div>	<div>Image not found</div> <div>Methylparaben</div> <div>Measured: 1.96</div> <div>Predicted: 2.06</div>	<div>Image not found</div> <div>Ethylparaben</div> <div>Measured: 2.47</div> <div>Predicted: 2.13</div>
<div>Image not found</div> <div>Ethyl 3-hydroxybenzoate</div> <div>Measured: 2.47</div> <div>Predicted: 2.14</div>		